

REMARKS/ARGUMENTS

Claims 5, 50 and 57 to 69 are pending in this application. Claims 5, 58 to 60 and 64 to 69 were withdrawn from consideration as being directed to a non-elected invention. Claims 50, 57 and 61 to 63 are presented for further prosecution.

Claim Objections

The Office Action has objected to claims 61 to 63 as allegedly depending from a canceled base claim, i.e., claim 56.

As amended herein, claims 61 to 63 are properly dependent from independent claim 50 which renders this objection moot. Applicants request reconsideration and removal of this objection.

Claim Rejections - 35 U.S.C. §112

The Action has rejected claims 50 and 57 under 35 U.S.C. §112, second paragraph, as allegedly being indefinite for reciting the term "information." Applicants respectfully disagree.

Applicants submit that claims 50 and 57 are not indefinite for reciting the term "information" based on the disclosure provided in the specification and the level of skill in the art. Throughout the specification and especially at paragraphs [0134] to [0140], Applicants have described what information is provided by or can be derived from an X-ray structure of a compound in association with a biological target molecule. This information includes but is not limited to computed deformation energy of binding information, volume overlap information, induced fit information, computed electrostatic interaction information, computed binding free energy information, computed energy minimization energy information, and computed molecular dynamics information.

Furthermore, the level of ordinary skill in the art is high. In the instant case, one of ordinary skill in the art is usually a scientist with an advanced degree and/or significant work experience in the field of computational, chemistry and/or biological areas. As such, based on the disclosure provided in the specification, one of skill in the art would readily be able to determine

what information to select from the structure to design a lead candidate. Therefore, claims 50 and 57 are not indefinite for reciting the term "information" because one of skill in the art, based on the disclosure provided in the specification and on their knowledge and experiences, would know which data, numbers or descriptors are meant by the term "information." Applicant's request reconsideration and removal of this rejection.

Claim Rejections - 35 U.S.C. §102

The Action has rejected claims 50 and 57 under 35 U.S.C. §102(b) as allegedly being anticipated by Dauter *et al.* Applicants respectfully disagree.

The invention, as defined by the claims, distinguishes over Dauter by claiming a method of designing a lead candidate having biophysical or biochemical activity against a biological target molecule.

Dauter does not disclose, teach or suggest any such methods. Instead, this publication discloses the use of halides for phasing macromolecular structures for X-ray crystallography. Phasing problems are well known in the art of X-ray crystallography. In fact, the determination of the structure of a molecule in a crystalline sample by X-ray crystallography requires knowing both the amplitude and the phase of the photon wave being diffracted from the sample. This publication provides a means for phasing macromolecular structures for X-ray crystallography but does not disclose, teach or suggest any methods for designing a lead candidate as required by the instant claims.

Dauter also discloses that the structure of an enzyme known as pepstatin-insensitive carboxylase (PCP) from *Pseudomonas sp. 101* was solved using crystals of PCP soaked in sodium bromide, lithium sulfate and glycerol in Tris buffer solutions. This protein was chosen because it was considered to be a good choice to showcase the use of bromine as a universal heavy atom. This publication, however, does not disclose, teach or suggest any methods for designing a lead candidate as required by the instant claims.


As explained above, Dauter is directed to a different field of art than the claimed invention. The cited publication discloses methods for phasing macromolecular structures for X-ray crystallography whereas the claimed invention is directed to methods for designing a lead

candidate having biophysical or biochemical activity against a biological target molecule. As such, Dauter does not anticipate the instant claims and claims 50 and 57 are novel over the disclosure of this publication. Applicants request reconsideration and removal of this rejection.

CONCLUSION

In view of the foregoing, Applicants believe all claims now pending in this Application are in condition for allowance. The issuance of a formal Notice of Allowance at an early date is respectfully requested. If the Examiner believes a telephone conference would expedite prosecution of this application, please telephone the undersigned at 858-350-6155.

Respectfully submitted,


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